Selective Nitrite Reduction at Heterobimetallic CoMg Complexes

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Supporting Information

1. ^{1}H, ^{13}C, and ^{31}P NMR Spectra

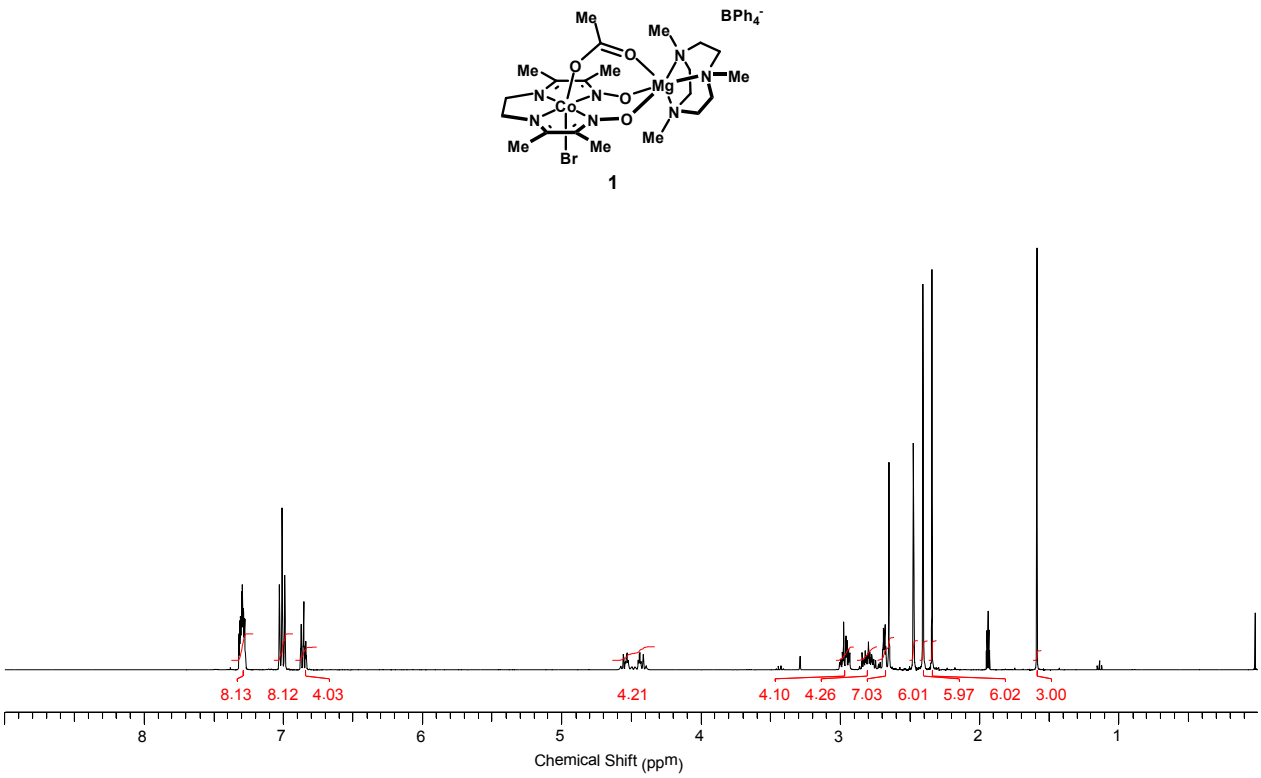


Figure S1. ^{1}H NMR spectrum of complex **1** (CD_3CN, room temperature).

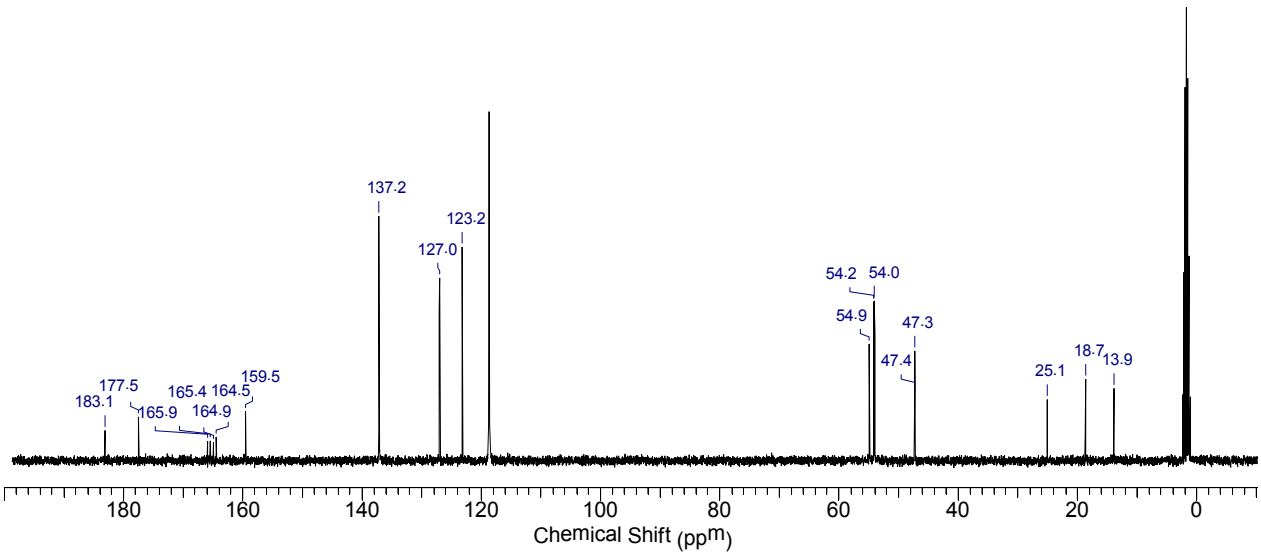


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of complex **1** (CD_3CN, room temperature).

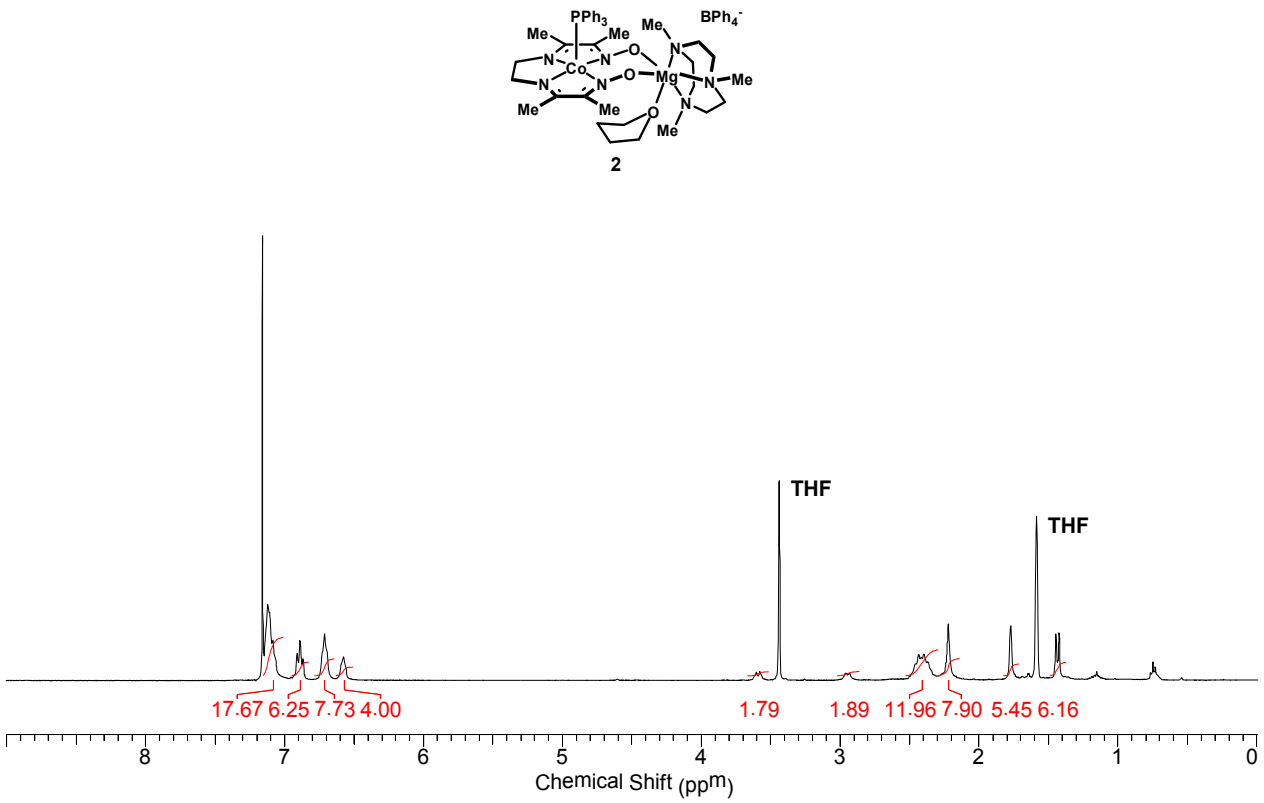


Figure S3. ^{1}H NMR spectrum of complex **2** (C_6D_6, room temperature).

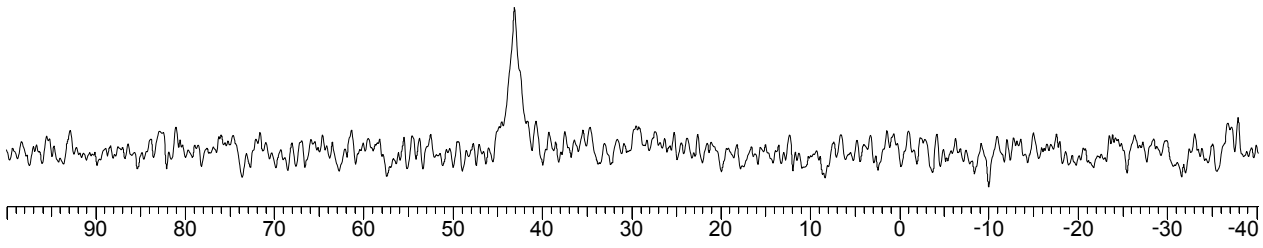


Figure S4. $^{31}P\{^{1}H\}$ NMR spectrum of complex **2** (C_6D_6, room temperature).

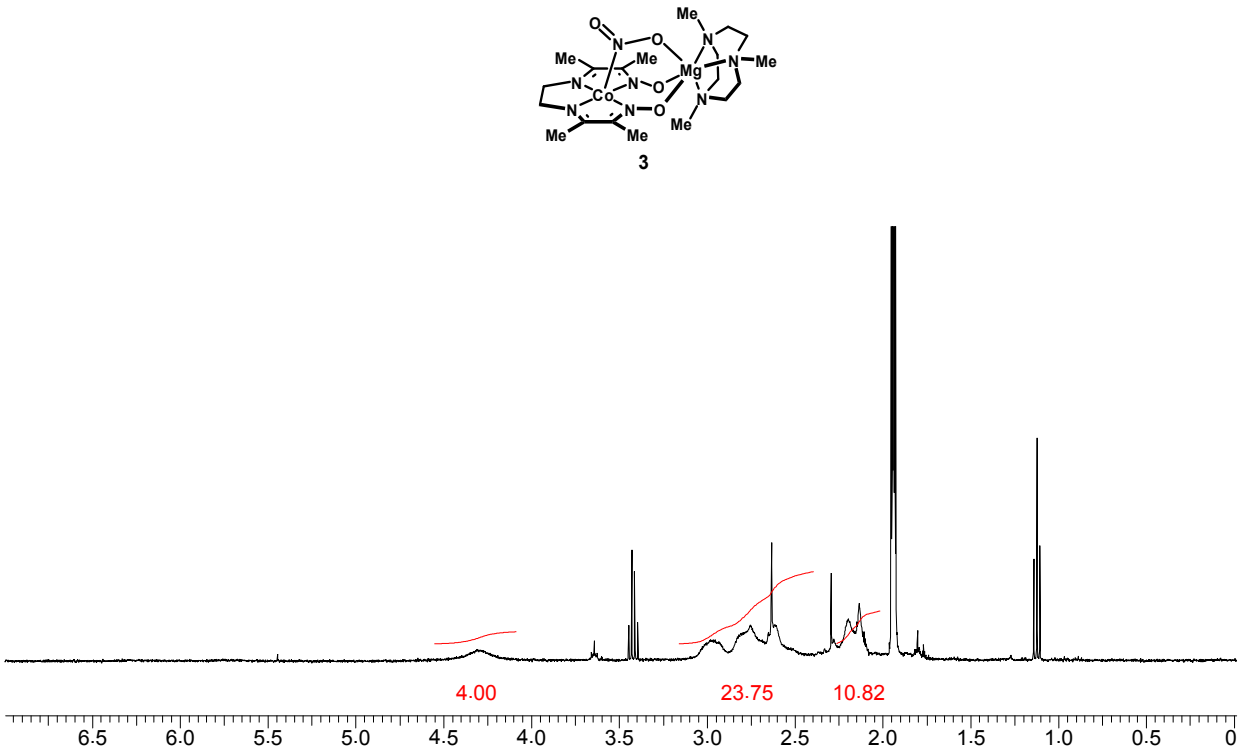


Figure S5. ^{1}H NMR spectrum of complex **3** (CD_3CN, room temperature).

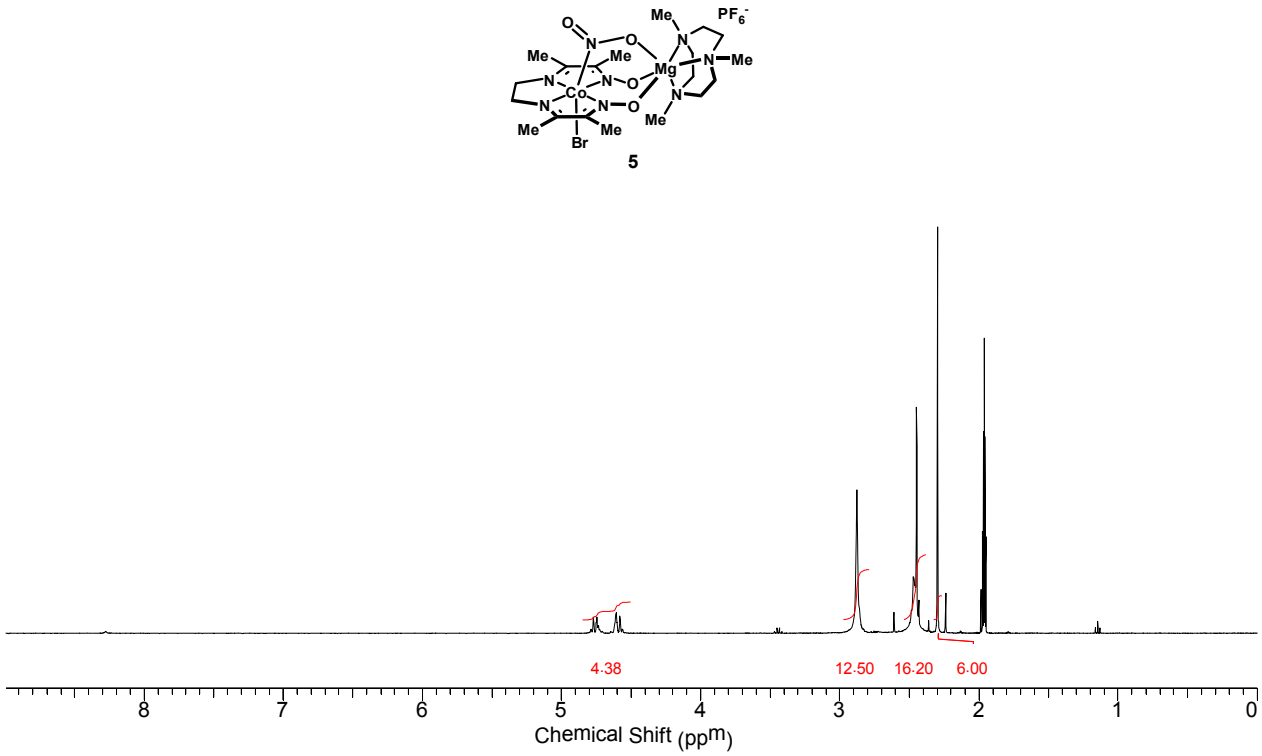


Figure S6. ^{1}H NMR spectrum of complex **5** (CD_3CN, room temperature).

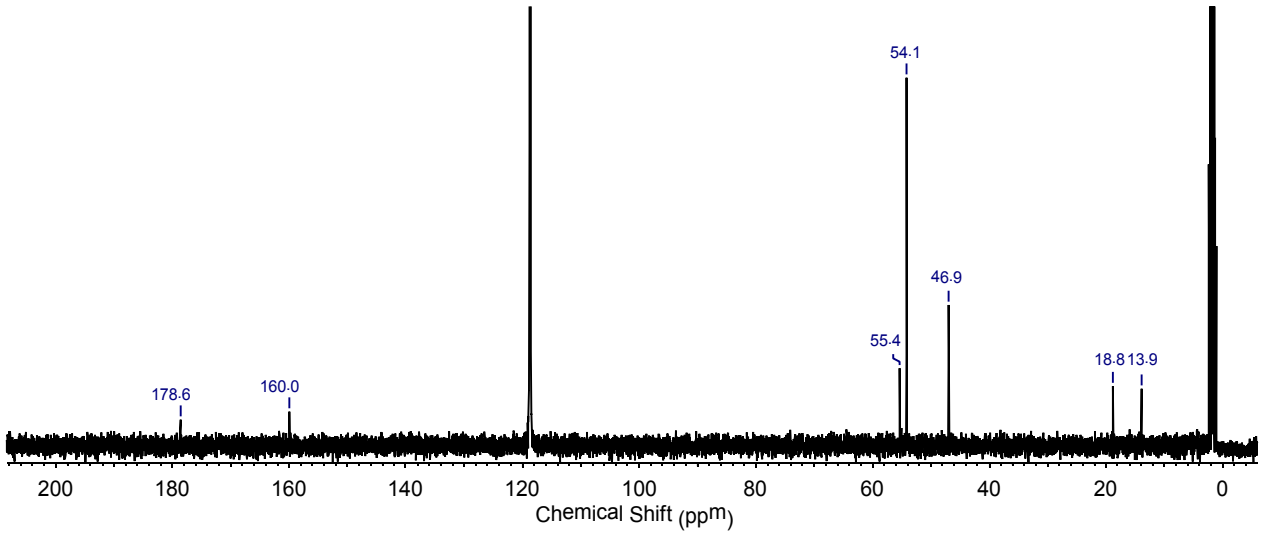


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of complex **5** (CD_3CN, room temperature).

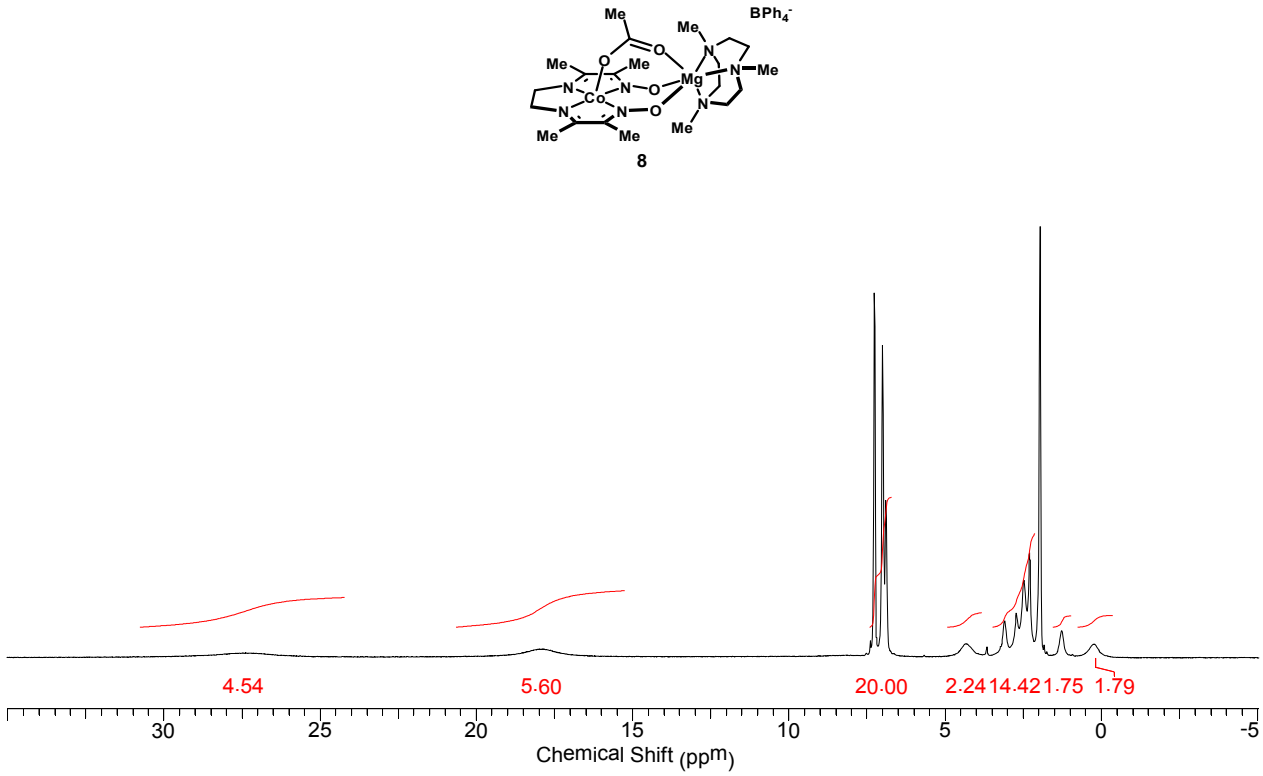


Figure S8. ^{1}H NMR spectrum of complex **8** (CD_3CN, room temperature).

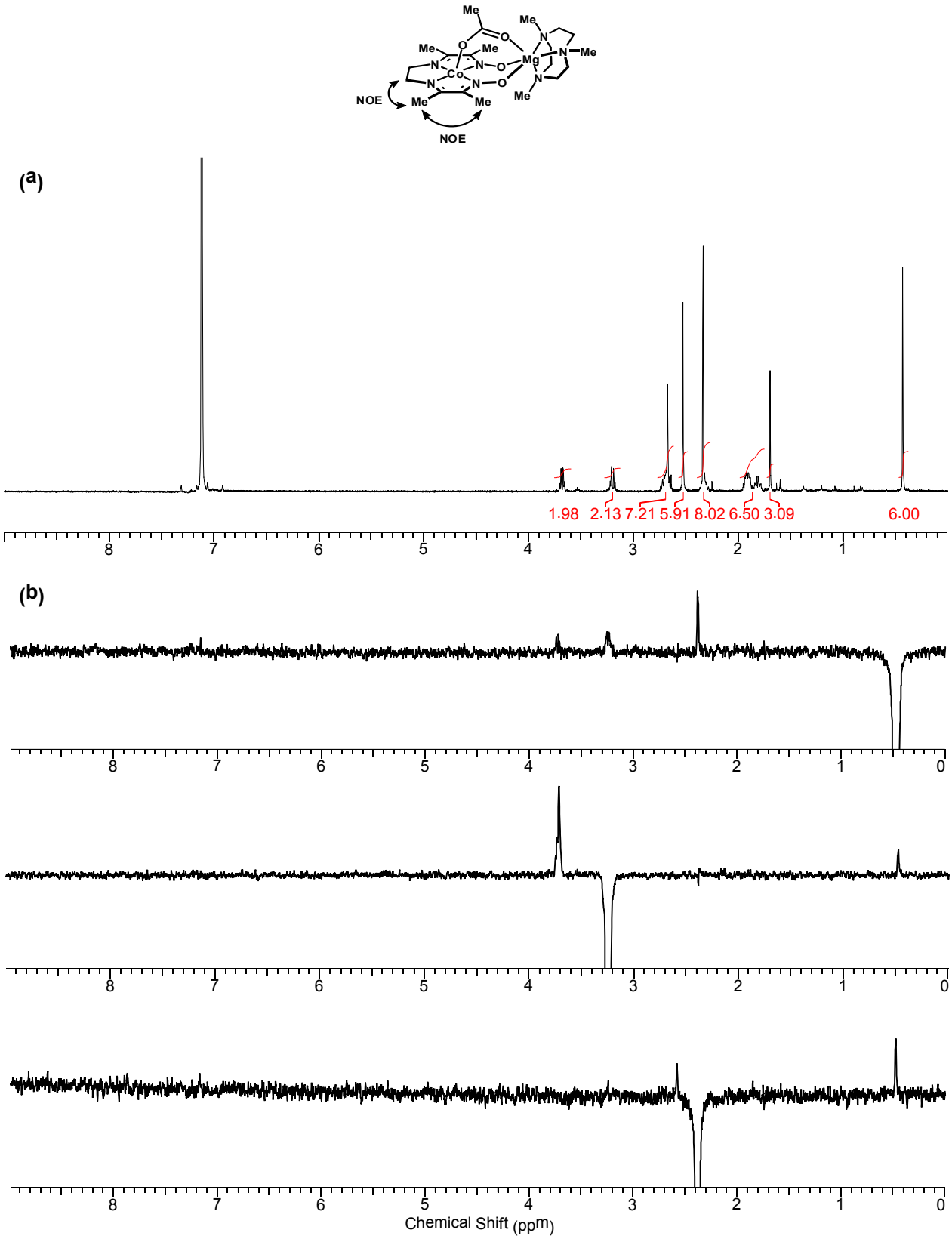


Figure S9. (a) ^{1}H NMR spectrum of [(μ-OAc)Co(doen)Mg(Me$_3$TACN)] (C_6D_6, room temperature). (b) NOE data for [(μ-OAc)Co(doen)Mg(Me$_3$TACN)].

2. Simulated EPR Spectra for *S* = ½ Complexes

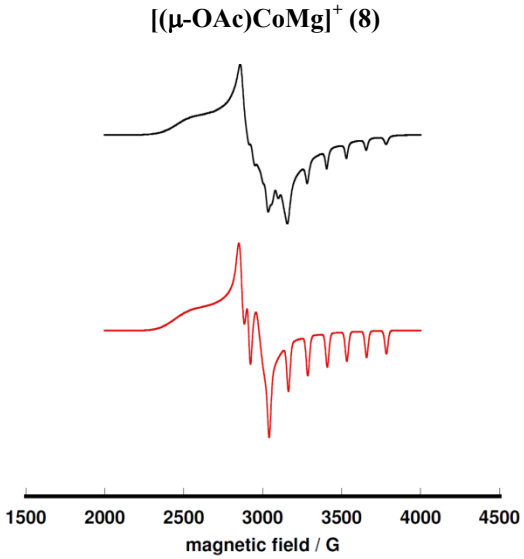


Figure S10. Experimental (black line, top) and simulated (red line, bottom) frozen solution (77 K) EPR spectra for [(μ-OAc)Co(^{Me}doen)Mg(Me$_3$TACN)]BPh$_4$. Simulated parameters: g_x = 2.550, g_y = 2.270, g_z = 2.030 (g_{max}–g_{min} = 0.52); A(Co)$_z$ = 350 MHz.

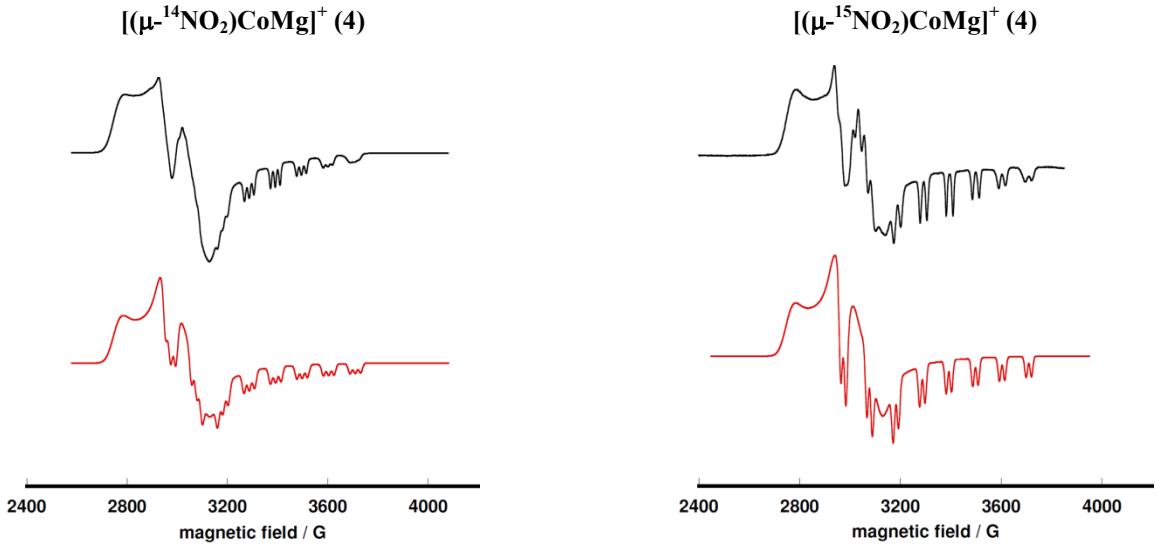


Figure S11. Experimental (black line, top) and simulated (red line, bottom) frozen solution (77 K) EPR spectra for [(μ-NO$_2$)Co(^{Me}doen)Mg(Me$_3$TACN)]BPh$_4$ using ^{14}NO$_2$ (left) and ^{15}NO$_2$ (right). Simulated parameters: g_x = 2.360, g_y = 2.190, g_z = 2.032 (g_{max}–g_{min} = 0.33); A(Co)$_z$ = 300 MHz, A(N)$_z$ = 60 MHz.

3. ATR-IR Spectra

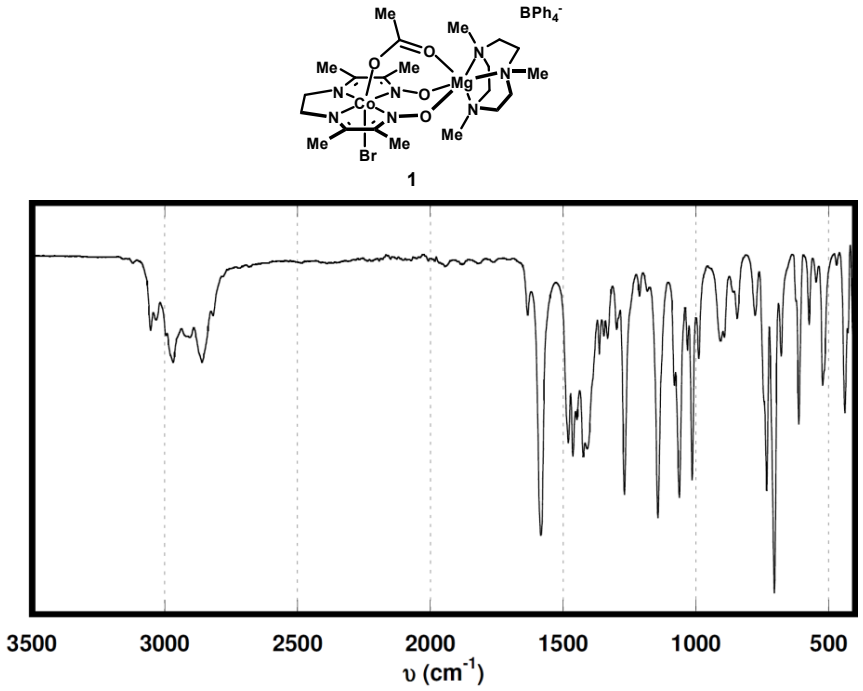


Figure S12. ATR-IR spectrum for a crystalline sample of complex **1**.

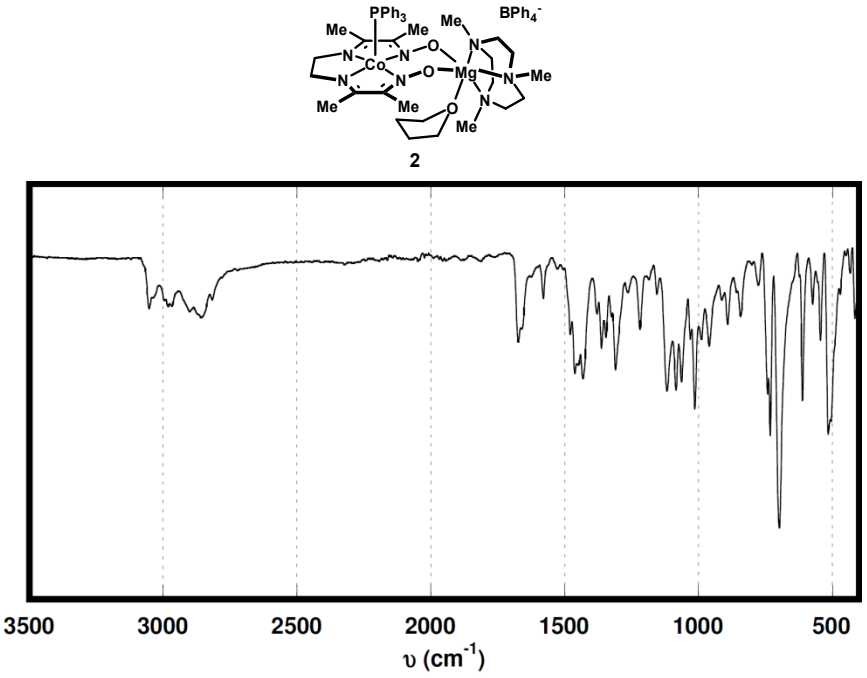


Figure S13. ATR-IR spectrum for a crystalline sample of complex **2**.

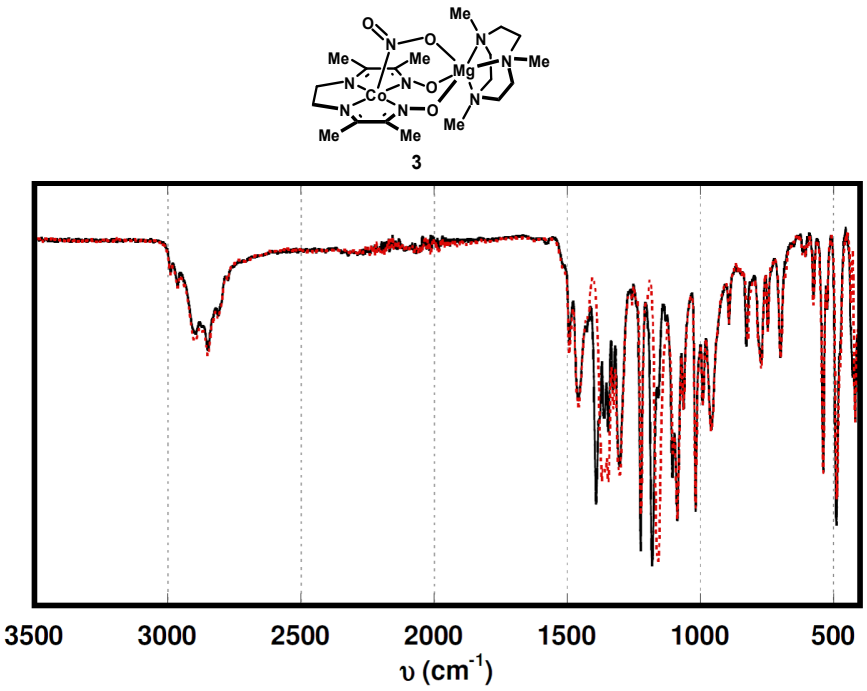


Figure S14. ATR-IR spectra for crystalline samples of complex **3** with $^{14}NO_2$ (black solid line) or $^{15}NO_2$ (red dotted line).

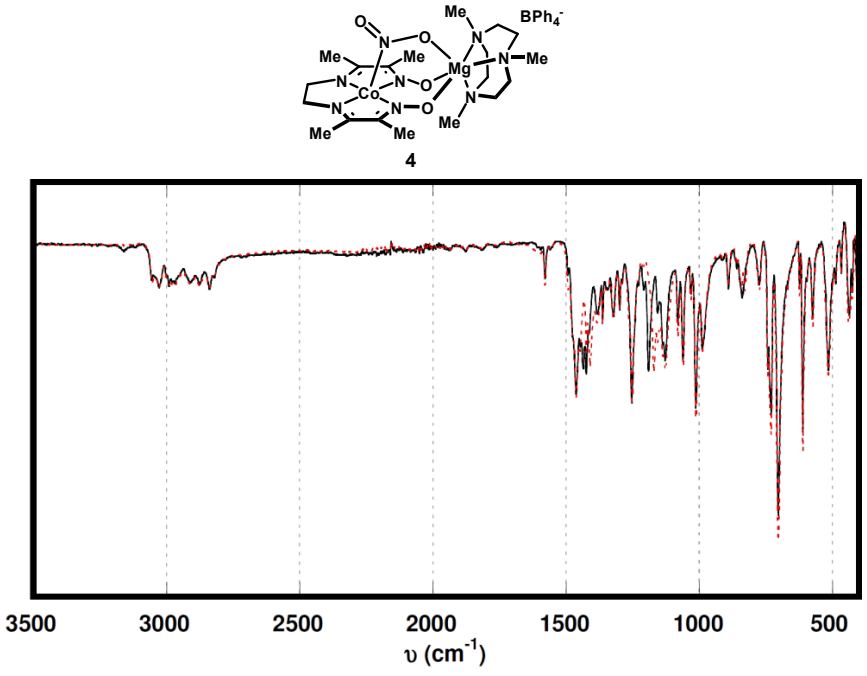


Figure S15. ATR-IR spectra for crystalline samples of complex **4** with $^{14}NO_2$ (black solid line) or $^{15}NO_2$ (red dotted line).

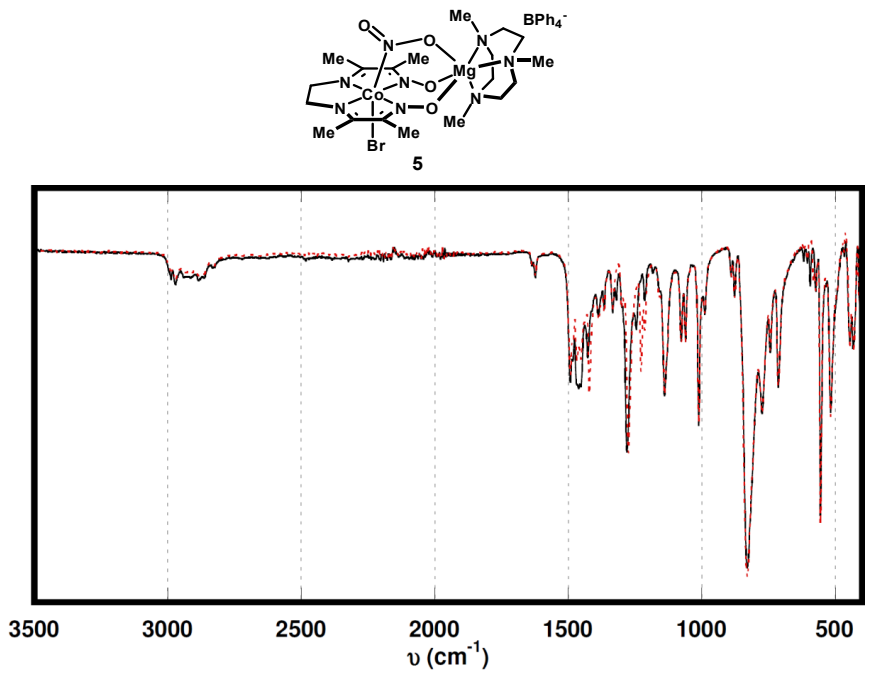


Figure S16. ATR-IR spectra for crystalline samples of complex **5** with $^{14}NO_2$ (black solid line) or $^{15}NO_2$ (red dotted line).

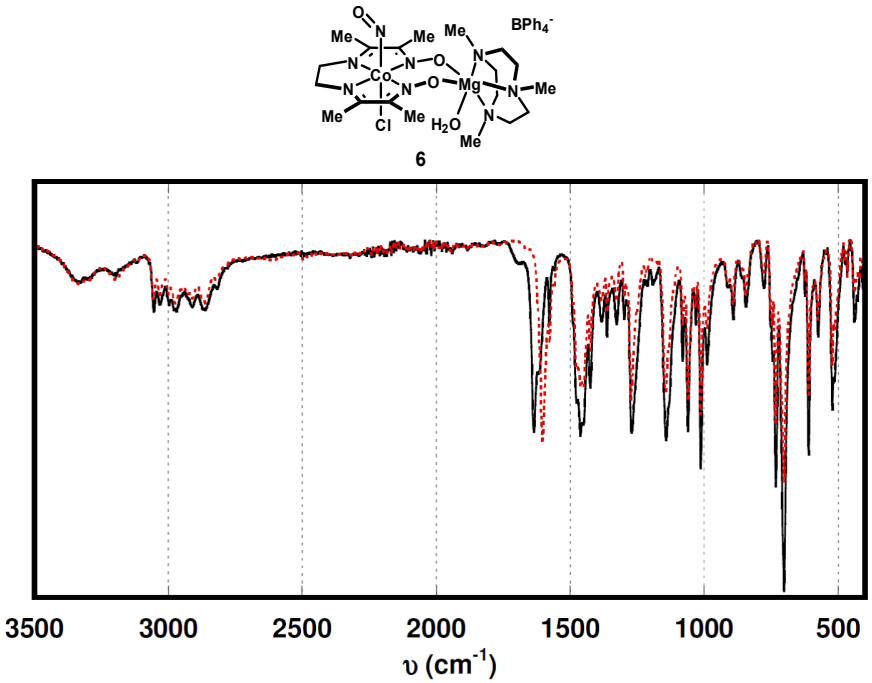


Figure S17. ATR-IR spectra for crystalline samples of complex **6** with $^{14}NO_2$ (black solid line) or $^{15}NO_2$ (red dotted line).

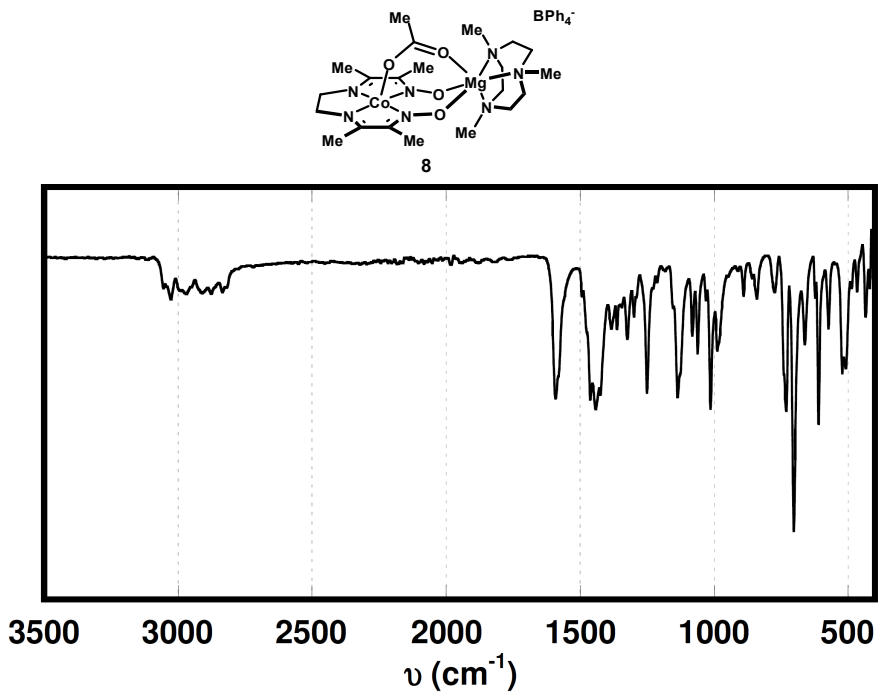


Figure S18. ATR-IR spectrum for a crystalline sample of complex **8**.

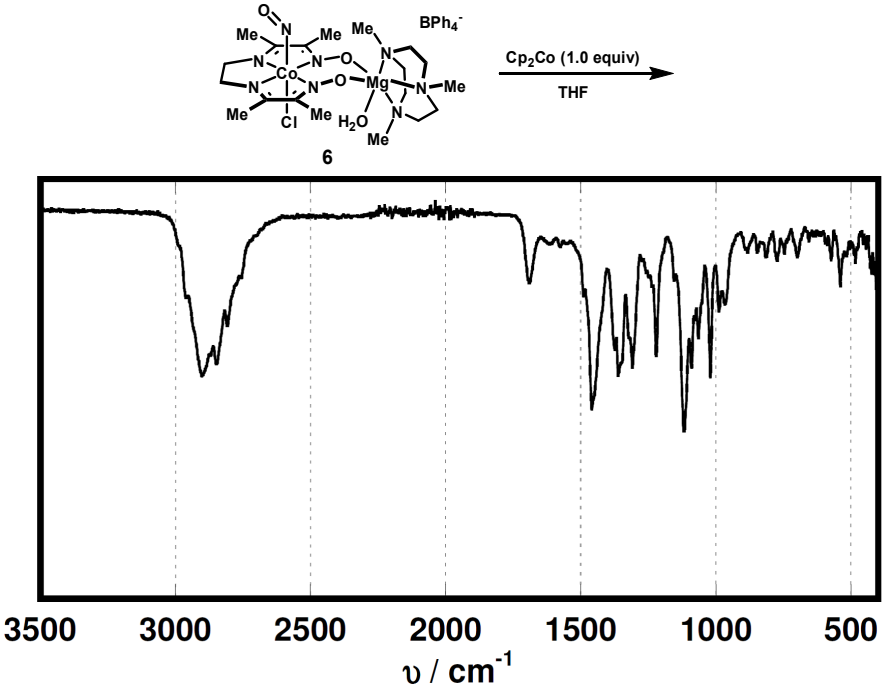


Figure S19. ATR-IR spectrum for the product mixture of a reaction between complex **6** and Cp_2Co (1.0 equiv).

4. UV-Vis Spectra

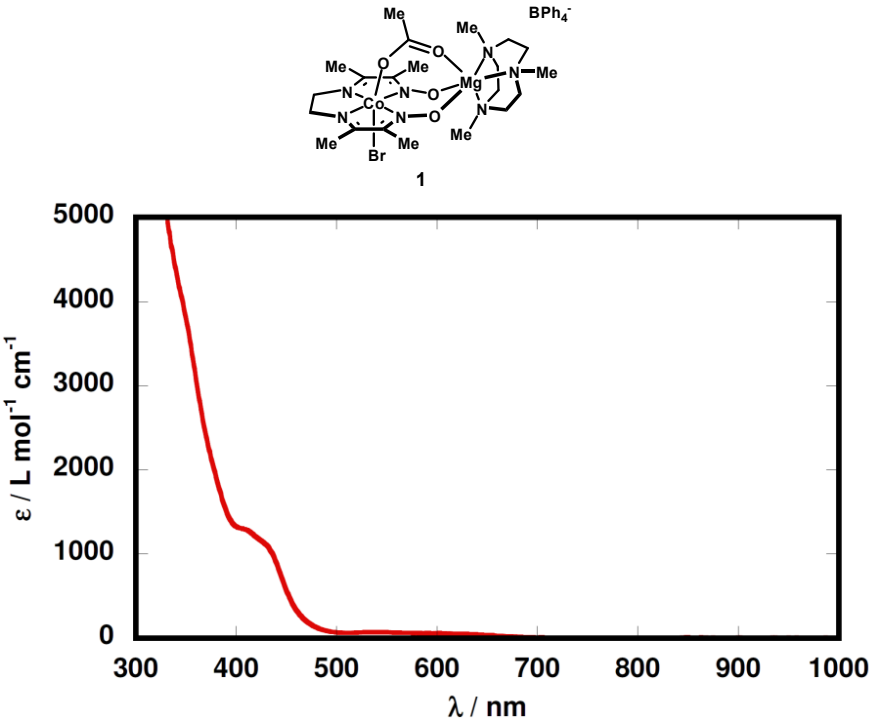


Figure S20. UV-Vis spectra of complex **1** (0.41 mM in MeCN, room temperature).

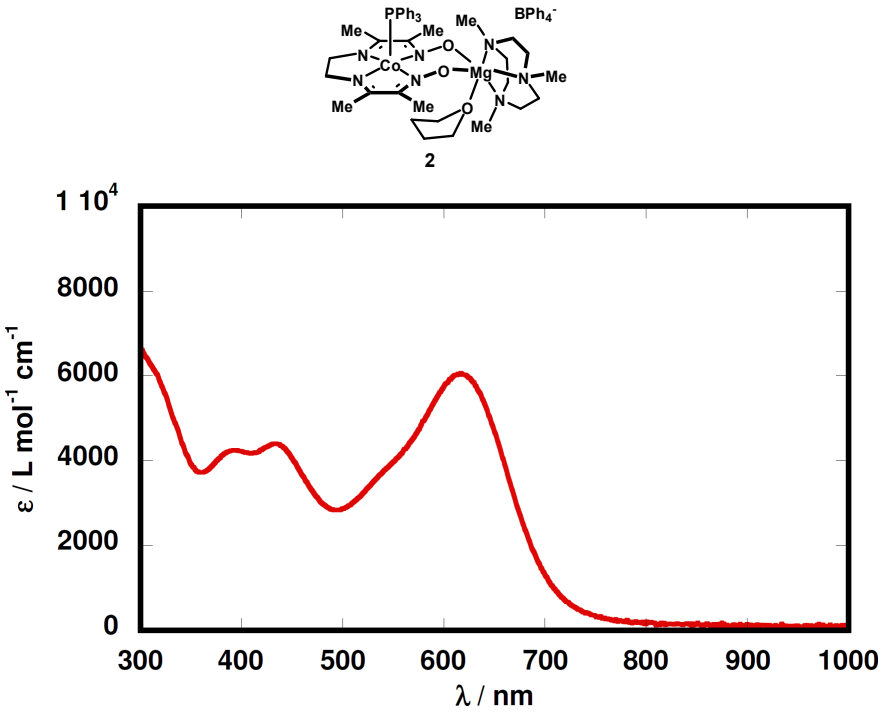


Figure S21. UV-Vis spectra of complex **2** (0.71 mM in MeCN, room temperature).

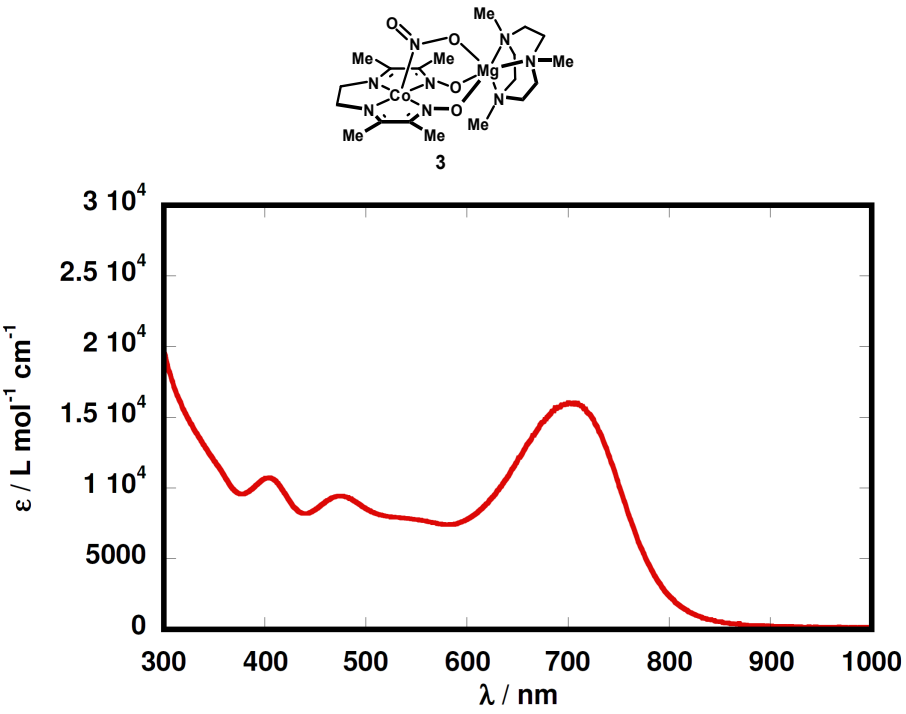


Figure S22. UV-Vis spectra of complex **3** (0.57 mM in C_6H_6, room temperature).

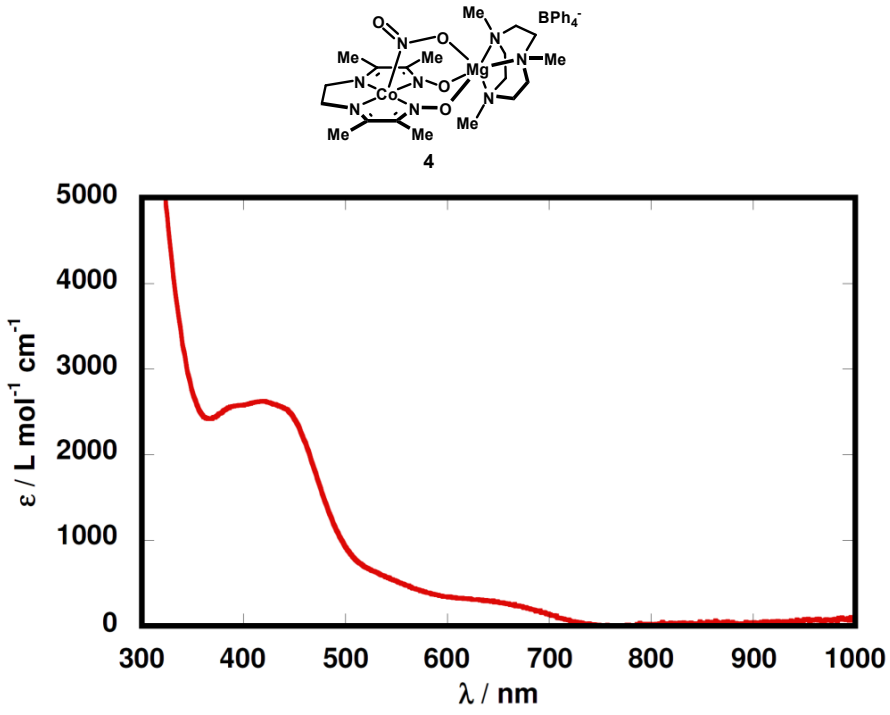


Figure S23. UV-Vis spectra of complex **4** (0.12 mM in MeCN, room temperature).

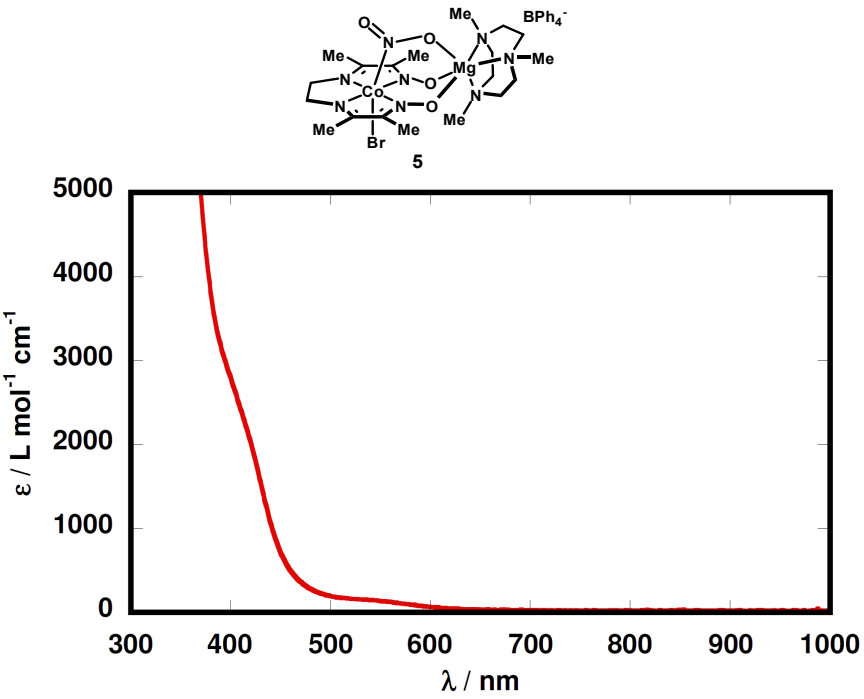


Figure S24. UV-Vis spectra of complex **5** (0.23 mM in MeCN, room temperature).

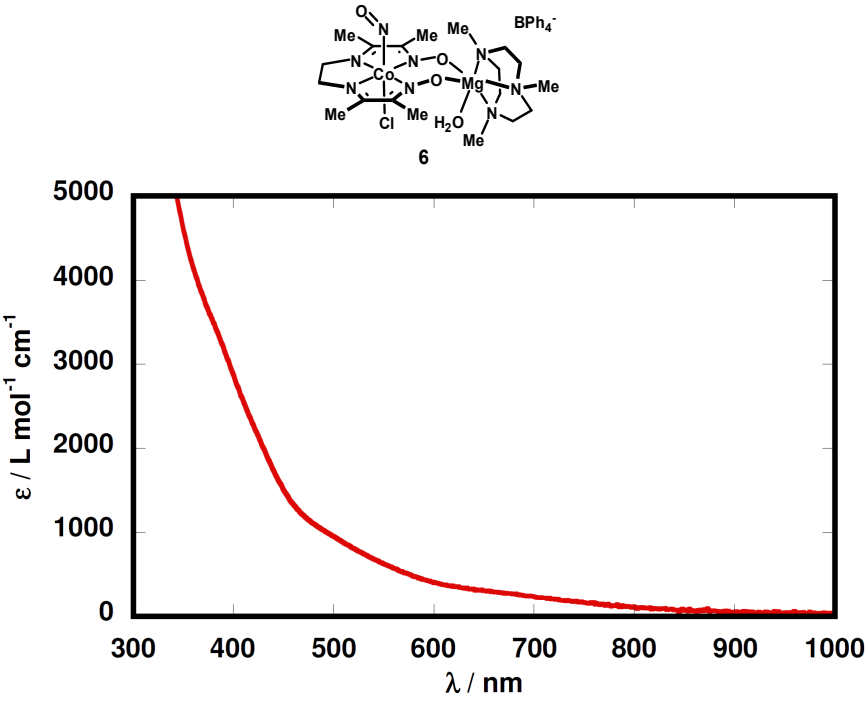


Figure S25. UV-Vis spectra of complex **6** (0.14 mM in MeCN, room temperature).

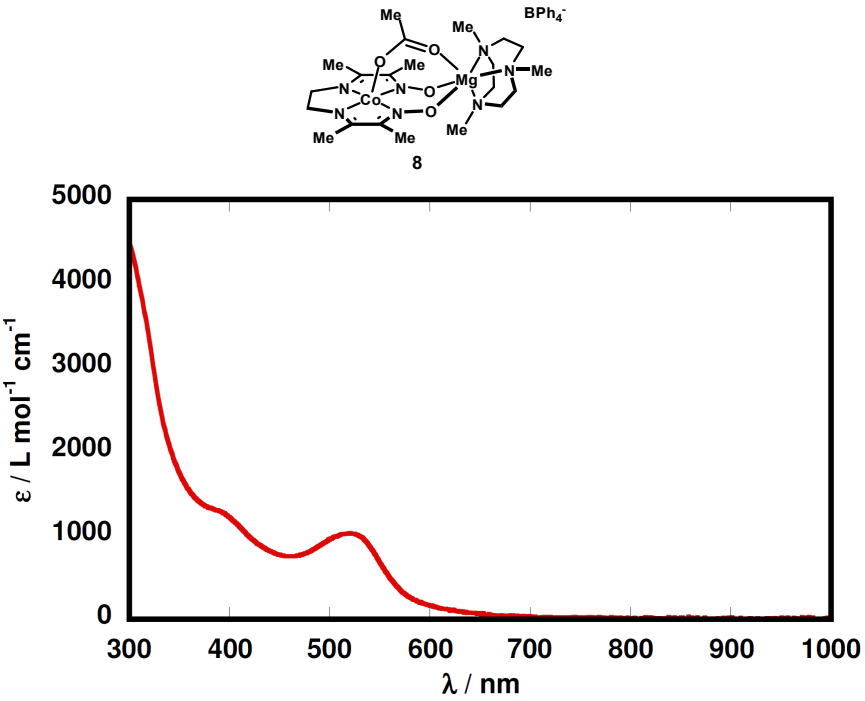


Figure S26. UV-Vis spectra of complex **8** (0.12 mM in THF, room temperature).

5. Reaction of $(PPh_3)Co(^{Me}doenH)$ (7) with $[n\text{-}Bu_4N][NO_2]$

88.4 mg of $Co(^{Me}doenH)Br_2$ (0.2 mmol, 1.0 eq), 57.7 mg of PPh_3 (0.22 mmol, 1.1 eq), and 83.2 mg of Cp_2Co (0.44 mmol, 2.2 eq) were taken up in 10 mL THF and stirred at room temperature for 1 h, during which time the solution turned dark purple. The reaction mixture was filtered through a short plug of Celite, and the filtrate was concentrated to dryness under reduced pressure. The solid material was washed with several portions of Et_2O to remove excess PPh_3 and Cp_2Co. After drying under vacuum, the $^{31}P\{^1H\}$ NMR spectrum of $(PPh_3)Co(^{Me}doenH)$ (**7**) (43 ppm) in the absence and presence of 1 eq of $[n\text{-}Bu_4N][NO_2]$ were compared.

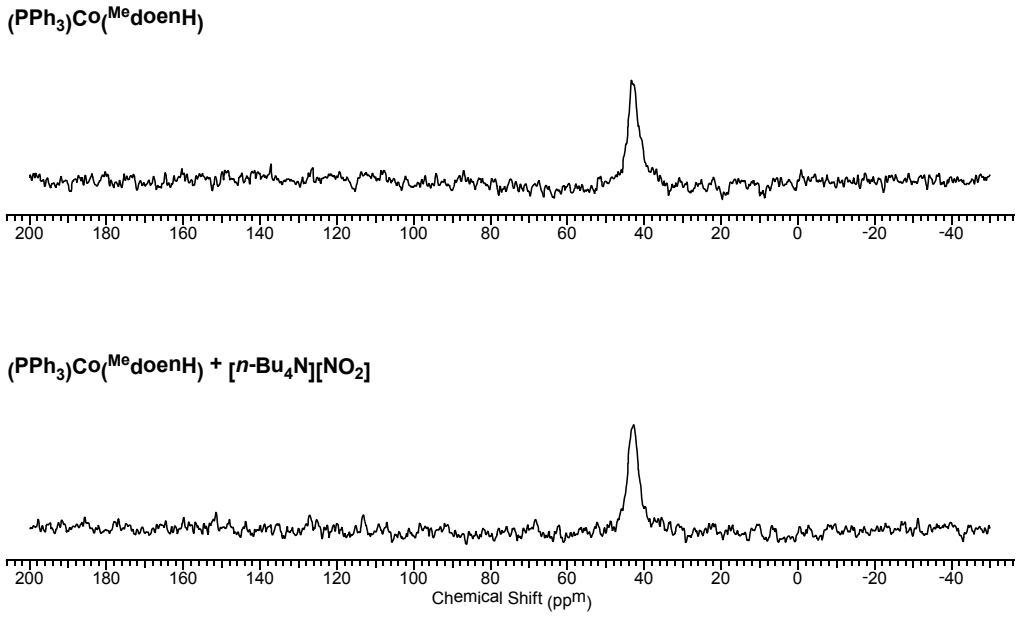


Figure S27. $^{31}P\{^1H\}$ NMR spectrum of complex **7** (THF, room temperature) in the absence (top) and presence of 1.0 eq $[n\text{-}Bu_4N][NO_2]$ (bottom).

6. Cyclic Voltammetry and Bulk Electrolysis Experiments

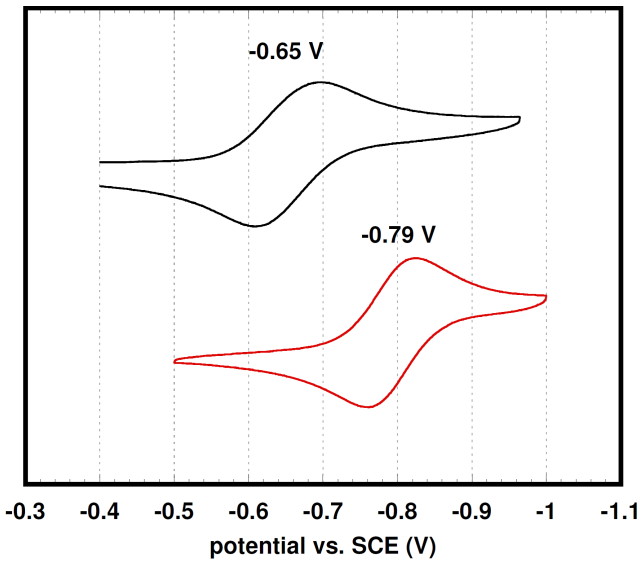


Figure S28. Cyclic voltammograms for 0.5 mM **6** (black line, top) and 0.5 mM **3** (red line, bottom). (100 mV/s scan rate; 0.1 M [n-Bu_4N][ClO_4] supporting electrolyte in MeCN; N_2 atmosphere; internally referenced to the Fc/Fc^+ reversible couple).

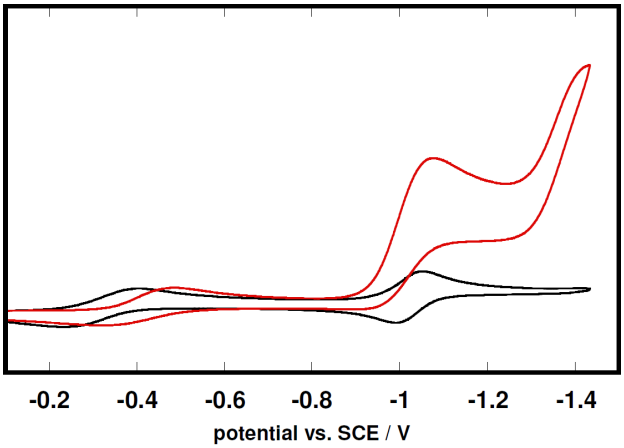
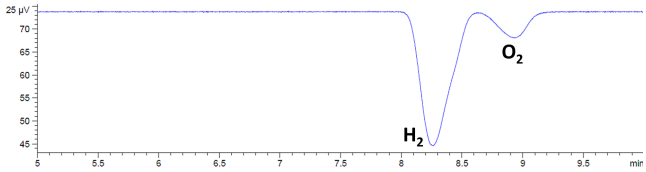


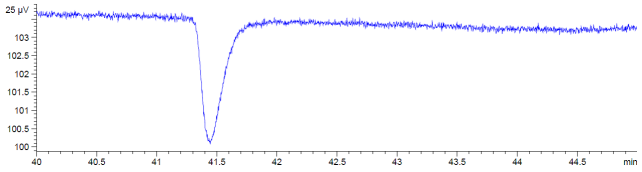
Figure S29. Cyclic voltammograms for 0.5 mM **1** in the absence (black line) and presence (red line) of 20 mM Et_3NHCl. (100 mV/s scan rate; 0.1 M [n-Bu_4N][ClO_4] supporting electrolyte in MeCN; N_2 atmosphere; internally referenced to the Fc/Fc^+ reversible couple).

Electrocatalytic hydrogen evolution activity of complex 1. Bulk electrolysis experiments were conducted with 0.5 mM **1** in the presence of 20 mM Et_3NHCl (2 h; –1.2 V vs. SCE; 0.1 M [n-Bu_4N][ClO_4] supporting electrolyte in MeCN; N_2 atmosphere). During electrolysis, the initially pale yellow solution turned red, which is the characteristic color of the [(μ-OAc)Co(II)Mg]$^+$ complex. After the 2-h period, the solution was exposed to air and the pale yellow color was restored. 96% Faradaic efficiency for hydrogen evolution was measured by GC analysis of the headspace. This yield accounts for the electron equivalent required to reduce the Co(III) pre-catalyst.

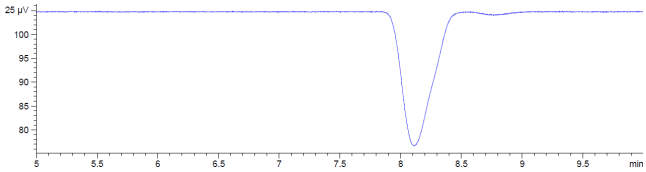
H_2 standard in air

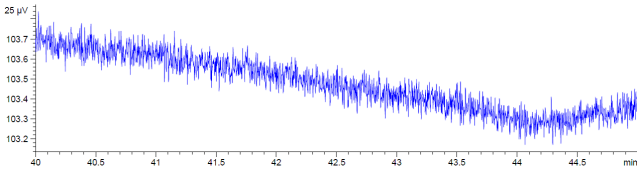


N_2O standard in air

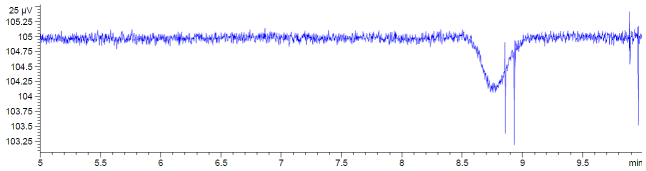


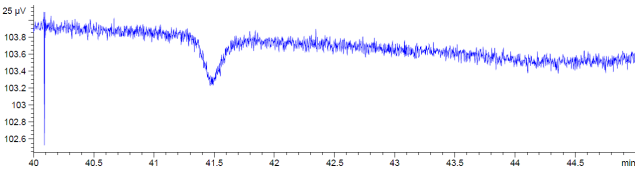
Bulk electrolysis (**1** + Et_3NHCl)



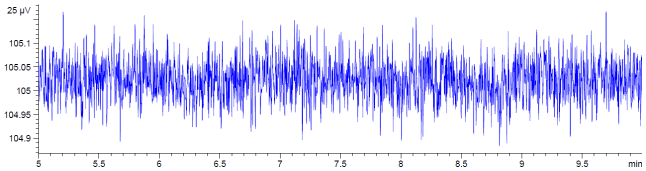


Bulk electrolysis (**1** + Et_3NHCl + [*n*-Bu_4N][NO_2])





Stoichiometric reduction and protonation of **6** (Cp_2Co; Et_3NHCl)



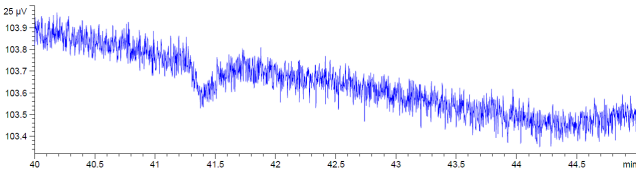


Figure S30. Gas chromatography traces indicating H_2 or N_2O formation for bulk electrolysis and stoichiometric reduction/protonation experiments. (N_2 carrier gas, 30 to 150 °C temperature gradient, HP-PLOT U and HP-PLOT Moleseive columns, thermal conductivity detector).

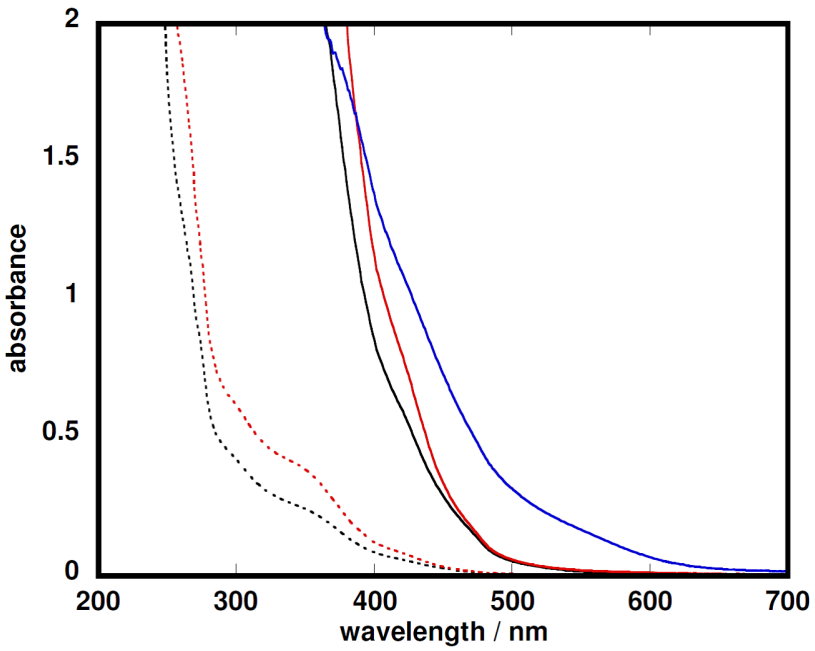
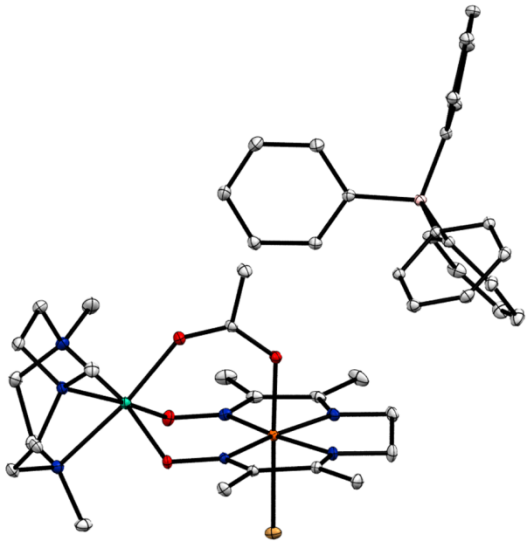
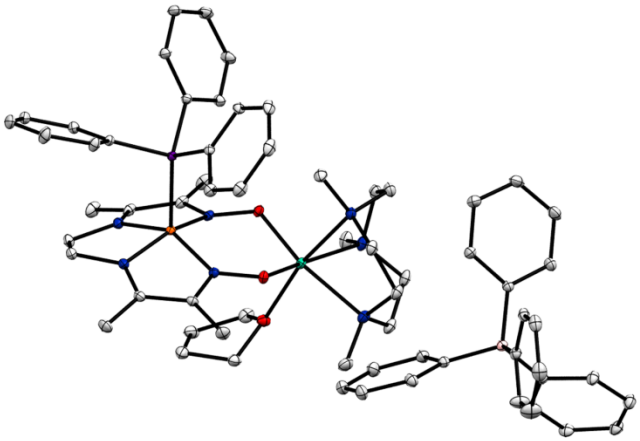


Figure S31. UV-Vis spectra of 0.5 mM complex **1**, 20 mM Et_3NHCl, and 20 mM [*n*-Bu_4N][NO_2] before bulk electrolysis (red solid line and red dotted line for 10-fold dilution). The UV-Vis spectrum after 2-h electrolysis at –1.2 V vs. SCE under an atmosphere of N_2 (blue solid line) and after exposure to air (black solid line and black dotted line for 10-fold dilution).

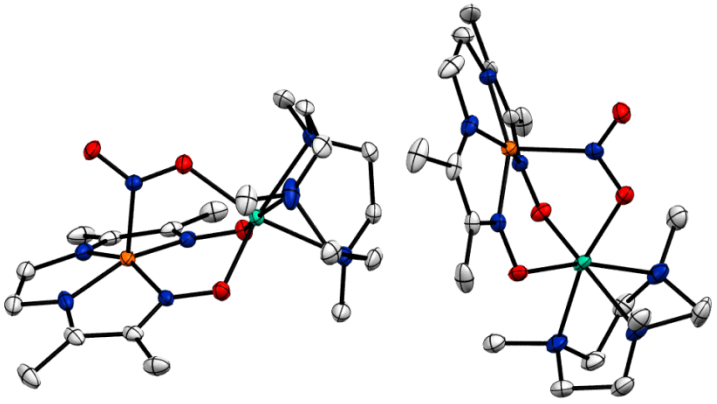
7. X-Ray Crystallography Data



Identification code	[(μ-OAc)(Br)Co(^{Me}doen)Mg(Me$_3$TACN)]BPh$_4$
Empirical formula	$C_{45}H_{60}BBrCoMgN_7O_4$
Formula weight	936.96
Temperature/K	373(2)
Crystal system	monoclinic
Space group	P21/c
a/Å	10.6455(5)
b/Å	15.5340(7)
c/Å	27.0655(12)
α/°	90.00
β/°	91.767(3)
γ/°	90.00
Volume/Å^3	4473.6(4)
Z	4
ρcalcmg/mm^3	1.391
m/mm^{-1}	1.342
F(000)	1960.0
Crystal size/mm^3	0.38 × 0.27 × 0.09
2Θ range for data collection	3.82 to 75.06°
Index ranges	-18 ≤ h ≤ 17, -26 ≤ k ≤ 26, -45 ≤ l ≤ 45
Reflections collected	166639
Independent reflections	22590[R(int) = 0.0492]
Data/restraints/parameters	22590/0/549
Goodness-of-fit on F2	1.033
Final R indexes [I>=2σ (I)]	R1 = 0.0353, wR2 = 0.0787
Final R indexes [all data]	R1 = 0.0545, wR2 = 0.0857
Largest diff. peak/hole / e Å^{-3}	0.76/-0.53

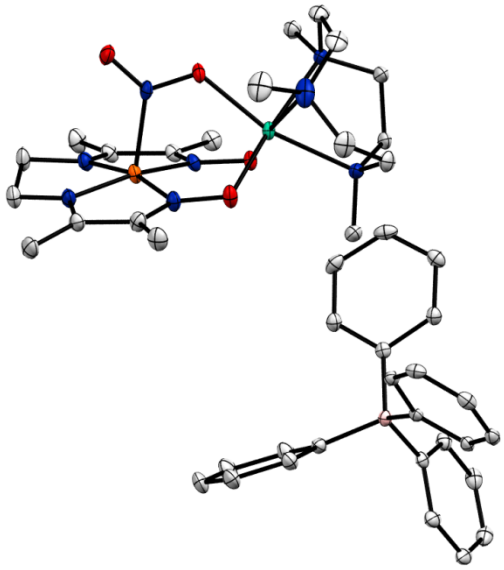


Identification code	[(PPh_3)Co(^{Me}doen)Mg(Me_3TACN)(THF)]BPh_4 - THF
Empirical formula	$C_{69}H_{88}BCoMgN_7O_4P$
Formula weight	1204.48
Temperature/K	373(2)
Crystal system	triclinic
Space group	P-1
a/Å	13.7524(8)
b/Å	14.0032(8)
c/Å	17.5215(10)
α/°	103.512(3)
β/°	99.587(3)
γ/°	100.736(3)
Volume/Å^3	3144.5(3)
Z	2
ρcalcmg/mm^3	1.272
m/mm^{-1}	0.363
F(000)	1284.0
Crystal size/mm^3	0.38 × 0.37 × 0.31
2Θ range for data collection	3.5 to 90.74°
Index ranges	-26 ≤ h ≤ 26, -28 ≤ k ≤ 27, -33 ≤ l ≤ 34
Reflections collected	373636
Independent reflections	49450[R(int) = 0.0548]
Data/restraints/parameters	49450/0/774
Goodness-of-fit on F2	1.030
Final R indexes [I>=2σ (I)]	R1 = 0.0428, wR2 = 0.1003
Final R indexes [all data]	R1 = 0.0813, wR2 = 0.1167
Largest diff. peak/hole / e Å^{-3}	0.69/-0.61



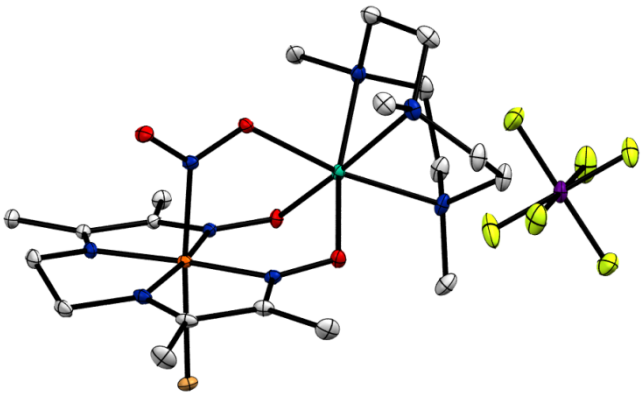
Identification code	(μ-NO_2)Co(^{Me}doen)Mg(Me_3TACN) - 2.5 THF
Empirical formula	$C_{29}H_{57}CoMgN_8O_{6.5}$
Formula weight	705.07
Temperature/K	373(2)
Crystal system	orthorhombic
Space group	Pnma
a/Å	22.7508(11)
b/Å	13.7761(8)
c/Å	22.5814(13)
α/°	90.00
β/°	90.00
γ/°	90.00
Volume/$Å^3$	7077.4(7)
Z	8
ρcalcmg/mm^3	1.323
m/mm^{-1}	0.555
F(000)	3024.0
Crystal size/mm^3	0.08 × 0.05 × 0.03
2Θ range for data collection	3.46 to 63.56°
Index ranges	$-32 \leq h \leq 20$, $-19 \leq k \leq 20$, $-33 \leq l \leq 32$
Reflections collected	93620
Independent reflections	11735[R(int) = 0.1087]
Data/restraints/parameters	11735/51/580
Goodness-of-fit on F2	1.084
Final R indexes [I>=2σ (I)]	R1 = 0.0881, wR2 = 0.1968
Final R indexes [all data]	R1 = 0.1577, wR2 = 0.2239
Largest diff. peak/hole / e $Å^{-3}$	1.10/-0.69

The structure was modeled with a 6% and 14% occupancy of the isomeric μ-(η^1-O:η^1-O)-NO_2 adduct.



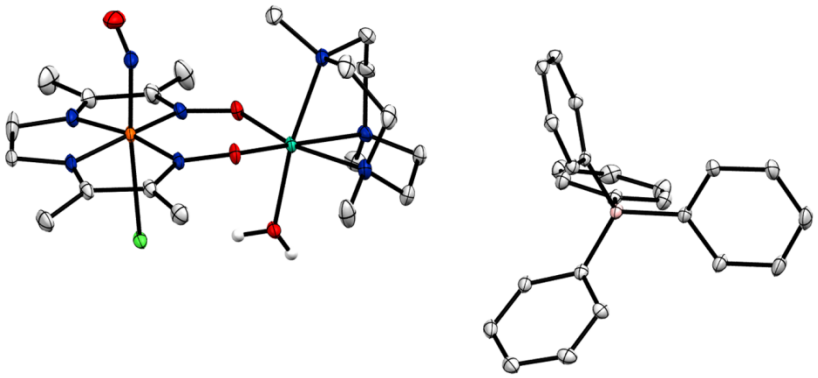
Identification code	[(μ-NO_2)Co(^{Me}doen)Mg(Me_3TACN)]BPh_4
Empirical formula	$C_{43}H_{57}BCoMgN_8O_4$
Formula weight	844.02
Temperature/K	373(2)
Crystal system	triclinic
Space group	P-1
a/Å	11.6227(13)
b/Å	11.9467(14)
c/Å	15.4979(18)
α/°	84.582(2)
β/°	79.196(2)
γ/°	83.448(2)
Volume/$Å^3$	2094.1(4)
Z	2
ρcalcmg/mm^3	1.339
m/mm^{-1}	0.477
F(000)	894.0
Crystal size/mm^3	0.37 × 0.25 × 0.21
2Θ range for data collection	2.68 to 58.18°
Index ranges	-15 ≤ h ≤ 15, -16 ≤ k ≤ 16, -20 ≤ l ≤ 21
Reflections collected	54074
Independent reflections	10342[R(int) = 0.0469]
Data/restraints/parameters	10342/18/595
Goodness-of-fit on F2	1.049
Final R indexes [I>=2σ (I)]	R1 = 0.0514, wR2 = 0.1271
Final R indexes [all data]	R1 = 0.0763, wR2 = 0.1427
Largest diff. peak/hole / e $Å^{-3}$	1.12/-0.29

The structure was modeled with a 14% occupancy of the bridging chloride complex [(μ-Cl)Co(^{Me}doen)Mg(Me_3TACN)]BPh_4

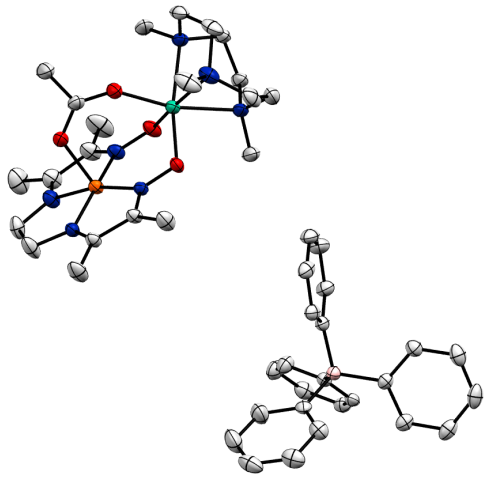


Identification code	[(μ-NO_2)(Br)Co(^{Me}doen)Mg(Me_3TACN)]PF_6
Empirical formula	$C_{19}H_{37}BrCoF_6MgN_8O_4P$
Formula weight	749.69
Temperature/K	373(2)
Crystal system	monoclinic
Space group	Pc
a/Å	8.5150(2)
b/Å	13.6712(4)
c/Å	12.9404(4)
α/°	90.00
β/°	94.8750(10)
γ/°	90.00
Volume/$Å^3$	1500.95(7)
Z	2
ρcalcmg/mm^3	1.659
m/mm^{-1}	2.055
F(000)	764.0
Crystal size/mm^3	0.36 × 0.27 × 0.21
2Θ range for data collection	2.98 to 78°
Index ranges	$-15 \le h \le 14$, $-23 \le k \le 23$, $-22 \le l \le 22$
Reflections collected	70619
Independent reflections	16686[R(int) = 0.0317]
Data/restraints/parameters	16686/2/378
Goodness-of-fit on F2	0.987
Final R indexes [I>=2σ (I)]	R1 = 0.0306, wR2 = 0.0674
Final R indexes [all data]	R1 = 0.0387, wR2 = 0.0700
Largest diff. peak/hole / e $Å^{-3}$	1.47/-0.29
Flack parameter	0.005(3)

The structure was modeled with a 13% occupancy of the *trans*-dinitro complex [(μ-NO_2)(NO_2)Co(^{Me}doen)Mg(Me_3TACN)]PF_6



Identification code	[(NO)(Cl)Co(^{Me}doen)Mg(Me_3TACN)(H_2O)]BPh_4 - THF
Empirical formula	$C_{47}H_{67}BClCoMgN_8O_5$
Formula weight	953.59
Temperature/K	373(2)
Crystal system	monoclinic
Space group	C2/c
a/Å	31.695(3)
b/Å	11.5842(12)
c/Å	30.376(4)
α/°	90.00
β/°	120.603(4)
γ/°	90.00
Volume/Å^3	9599.4(19)
Z	8
ρcalcmg/mm^3	1.320
m/mm^{-1}	0.480
F(000)	4048.0
Crystal size/mm^3	0.34 × 0.27 × 0.04
2Θ range for data collection	3.82 to 74.74°
Index ranges	-52 ≤ h ≤ 53, -19 ≤ k ≤ 19, -51 ≤ l ≤ 50
Reflections collected	150910
Independent reflections	23710[R(int) = 0.0652]
Data/restraints/parameters	23710/0/602
Goodness-of-fit on F2	1.017
Final R indexes [I>=2σ (I)]	R1 = 0.0521, wR2 = 0.1177
Final R indexes [all data]	R1 = 0.0988, wR2 = 0.1377
Largest diff. peak/hole / e Å^{-3}	0.84/-0.68



Identification code	[(μ-OAc)Co(^{Me}doen)Mg(Me_3TACN)]BPh_4 - THF
Empirical formula	$C_{53}H_{76}BCoMgN_7O_6$
Formula weight	1001.26
Temperature/K	373(2)
Crystal system	triclinic
Space group	P-1
a/Å	14.2031(6)
b/Å	14.4679(7)
c/Å	15.6818(7)
α/°	70.548(2)
β/°	68.324(2)
γ/°	63.304(2)
Volume/$Å^3$	2620.6(2)
Z	2
ρcalcmg/mm^3	1.269
m/mm^{-1}	0.395
F(000)	1070.0
Crystal size/mm3	0.19 × 0.14 × 0.11
2Θ range for data collection	3.32 to 66.12°
Index ranges	$-21 \le h \le 21$, $-21 \le k \le 22$, $-23 \le l \le 23$
Reflections collected	76411
Independent reflections	17965[R(int) = 0.0855]
Data/restraints/parameters	17965/0/640
Goodness-of-fit on F2	1.028
Final R indexes [I>=2σ (I)]	R1 = 0.0692, wR2 = 0.1651
Final R indexes [all data]	R1 = 0.1566, wR2 = 0.2028
Largest diff. peak/hole / e $Å^{-3}$	1.24/-0.80

8. Computational methods and optimized geometries

Computational Methods. Geometry optimizations were performed using the Gaussian03 package.[1] The B3LYP exchange-correlation functional was employed with a 6-31G(d) basis set. A full frequency calculation was performed on each structure in order to verify the absence of negative vibrational frequencies.

	(μ-NO_2)CoMg	**[(μ-NO_2)CoMg]$^+$**	**[(μ-NO_2)(Cl)CoMg]$^+$**
Co–N(NO_2)	1.933	2.017	1.926
Mg–O(NO_2)	2.065	2.071	2.125
Co–N(oxime)	1.895, 1.893	1.917, 1.917	1.932, 1.926
Co–N(imine)	1.855, 1.855	1.885, 1.873	1.882, 1.880
Σ N–Co–N	351.1	355.3	360.0
N–O(Mg)	1.298	1.290	1.273
N–O(terminal)	1.223	1.218	1.215
C–N(oxime)	1.342, 1.339	1.324, 1.323	1.317, 1.315
C–N(imine)	1.328, 1.324	1.306, 1.303	1.296, 1.294
C(oxime)–C(imine)	1.429, 1.432	1.462, 1.466	1.467, 1.471
N–O(oxime)	1.342, 1.336	1.307, 1.306	1.300, 1.302

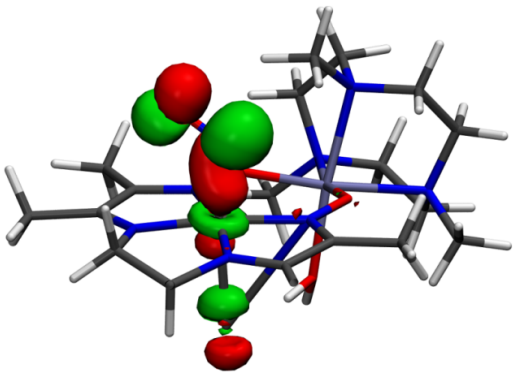
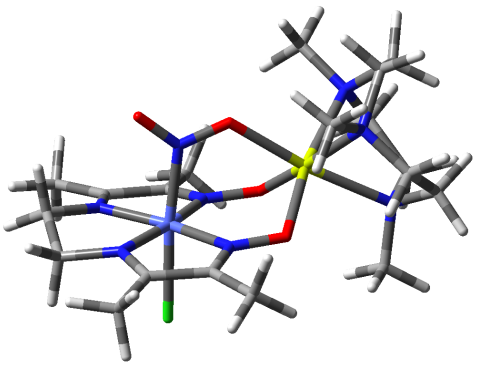


Figure S32. Isosurface representation of the HOMO for [(NO)(Cl)Co(^{Me}doen)Mg(Me_3TACN)(H_2O)]$^+$

[1] Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

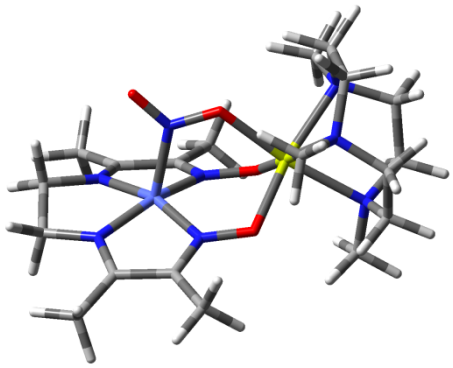


[(μ-NO_2)CoMg]$^+$

Z **= 1,** ***m*** **= 1**

E = –3528.07186570

N	2.99441800	1.32383800	-0.40476900
C	2.68437600	2.54695900	-0.11735800
N	0.66189700	1.56555600	0.46680200
C	1.31762200	2.70348200	0.40389500
N	0.69438200	-1.57311500	0.43897100
C	1.37722400	-2.69647700	0.36021000
N	3.06064400	-1.25667400	-0.32930500
C	2.77197300	-2.48781600	-0.04489200
C	4.39015500	-0.66714600	-0.51945500
H	4.99548700	-1.23809300	-1.23103600
H	4.89494300	-0.66356400	0.45300300
C	4.20521300	0.78015400	-1.02215300
H	4.04745600	0.77816200	-2.10639500
H	5.09508800	1.37496500	-0.79660900
C	0.76323600	-4.02357700	0.68213600
H	1.52303200	-4.76183700	0.94778300
C	3.75423300	-3.62077500	-0.06502200
H	3.96643200	-3.94601700	0.96154300
C	0.68022900	4.00017100	0.79418400
H	1.41400600	4.80457400	0.86954700
C	3.58200200	3.73425500	-0.30405700
H	3.10203000	4.48215000	-0.94505700
O	-0.59707000	1.54703800	0.79774900
O	-0.57374700	-1.59074000	0.72484800
N	-3.21677200	1.43924900	-0.80336300
N	-3.22128600	-0.04998400	1.60102300
N	-3.06050900	-1.45805600	-1.00141500
C	-3.52987500	2.19925300	0.42908600
H	-2.63258800	2.77473300	0.66389200
H	-4.35286800	2.91209200	0.26131200
C	-3.88038300	1.29234800	1.63608300
H	-4.96514900	1.16696200	1.72547400
H	-3.56283900	1.81744600	2.54093900
C	-3.68521400	-2.10842100	0.17986000
H	-2.91217400	-2.75208100	0.60844700
H	-4.52151500	-2.75847100	-0.12549500
C	-4.18595600	-1.14484700	1.26561400
H	-4.39947000	-1.73937600	2.16316200
H	-5.13985300	-0.70690700	0.96921500
C	-3.99188400	-0.69288200	-1.86908300
H	-3.47263200	-0.54775000	-2.82124500
H	-4.90113400	-1.27528900	-2.08706800
C	-4.38883600	0.68316500	-1.31596100
H	-4.89302400	1.24567200	-2.11392100
H	-5.12193200	0.58279400	-0.51692100
C	-2.52677300	-0.33926800	2.88262300
H	-1.75188900	0.41184500	3.04908700
H	-3.22839100	-0.34142700	3.72902000
H	-2.03586200	-1.31171700	2.81413200
C	-2.67455200	2.33982200	-1.84219600
H	-2.43199400	1.76433000	-2.73862200
H	-3.39211300	3.13082500	-2.10672200
H	-1.75397300	2.79855600	-1.47508400
C	-2.39358900	-2.50043800	-1.81736400
H	-1.67306300	-3.03040500	-1.19300500
H	-3.11847500	-3.22123600	-2.22385300
H	-1.85614900	-2.02698000	-2.64140900
H	0.19164600	-4.42188300	-0.16656600
H	4.69783000	-3.33609900	-0.53269900
H	3.34565700	-4.48161800	-0.60362900
H	4.53665900	3.46156100	-0.75504100
H	3.77972900	4.21106600	0.66320300
H	0.18009900	3.88973500	1.76170100
H	-0.08456200	4.30299400	0.06757000
H	0.07147800	-3.91409200	1.52159600
Co	1.72624000	0.01400900	0.05426600
Mg	-1.65014300	-0.01060500	-0.03724300
O	-0.37417700	0.02429800	-1.73587300
Cl	2.49175200	0.02863100	2.21106100
O	1.53298200	-0.00037600	-2.72107600
N	0.89785400	0.00878000	-1.68489100

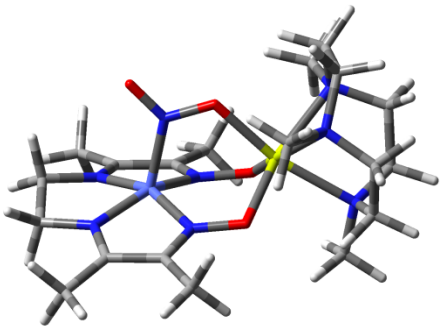


[(μ-NO_2)CoMg]$^+$

***Z* = 1, *m* = 2**

E = –3067.84380395

N	3.25125800	1.28138400	0.12042700
N	0.84886500	1.55768400	-0.53375800
C	1.54899400	2.67813300	-0.61850800
N	0.87960000	-1.48782800	-0.66785400
C	1.59021600	-2.59767600	-0.78811100
N	3.21280700	-1.26022200	0.18807100
C	2.96287000	-2.44371100	-0.29708800
C	4.41942200	-0.73241800	0.82134700
H	5.31864500	-1.31812600	0.60617100
H	4.24636500	-0.74817900	1.90424600
C	4.59457600	0.73025700	0.34883200
H	5.16498900	0.75736500	-0.58866200
H	5.15008000	1.30375500	1.09974100
O	-0.44001500	1.59475800	-0.74603700
O	-0.39445800	-1.50451400	-0.95568500
O	-0.41890500	-0.11108200	1.75140900
N	-3.11325600	1.34507100	0.97508500
N	-3.05900500	-1.47668100	0.77194400
N	-2.94687200	0.09410800	-1.69538200
C	-3.74609700	0.57450100	2.08824100
H	-3.42782900	1.00368800	3.04211900
H	-4.83446100	0.69927800	2.05041000
C	-3.36480100	-0.92454100	2.11172200
H	-4.16952400	-1.49344600	2.60483800
H	-2.45689200	-1.05142400	2.70496800
C	-3.85058000	-1.07823400	-1.58058400
H	-3.31265500	-1.91900300	-2.02871200
H	-4.76860900	-0.93298400	-2.17261300
C	-4.23200400	-1.46116900	-0.14013400
H	-4.71327900	-2.44869000	-0.16589600
H	-4.98285200	-0.77948600	0.25742300
C	-3.59186000	1.41777500	-1.51507700
H	-2.83024000	2.15883200	-1.77443700
H	-4.43037200	1.54837100	-2.21921200
C	-4.09575800	1.69915900	-0.09440600
H	-4.34685400	2.76661000	-0.03483000
H	-5.03153500	1.16808000	0.08319500
C	-2.51317400	-2.84315400	0.90704000
H	-1.59345700	-2.80562700	1.49541100
H	-3.23062400	-3.51512900	1.40206300
H	-2.26959700	-3.23857100	-0.08067300
C	-2.45061700	2.56609900	1.49097700
H	-1.98436100	3.09690300	0.65930400
H	-3.16562500	3.23289200	1.99550700
H	-1.66545100	2.27755800	2.19318700
C	-2.27232200	0.06894300	-3.01489000
H	-1.71928700	-0.86620100	-3.11743900
H	-2.99378400	0.16191500	-3.84049800
H	-1.55900500	0.89383600	-3.06362600
O	1.42930300	-0.18875400	2.83748700
C	2.96266600	2.48239200	-0.30306000
C	0.91111600	3.97926700	-0.99460300
H	0.25904600	4.34384600	-0.19076700
H	1.65511000	4.75085300	-1.20216500
H	0.28146600	3.84997000	-1.88099000
C	3.96449200	3.58736300	-0.47597100
H	3.96486300	3.95230200	-1.50966900
H	3.70826300	4.43900400	0.16530300
H	4.97621900	3.26559600	-0.22430600
C	0.98781100	-3.86529100	-1.30980000
H	1.74858900	-4.61810300	-1.52543300
H	0.28059700	-4.29217500	-0.58739400
H	0.42296000	-3.66433900	-2.22589000
C	3.93381300	-3.58827100	-0.33582400
H	3.56119600	-4.42225900	0.27070600
H	4.05062700	-3.96118200	-1.35953700
H	4.91748200	-3.30909000	0.04382000
Mg	-1.49387200	-0.02472700	-0.01648300
Co	1.85691700	0.01836400	0.00345100
N	0.87081900	-0.09716700	1.75874600



[(μ-NO_2)CoMg]

***Z* = 0, *m* = 1**

E = –3067.98594541

N	3.18995500	1.26504900	0.05246200
N	0.84035200	1.52471200	-0.57814800
C	1.51795700	2.68235500	-0.60407800
N	0.88784800	-1.45533400	-0.70485300
C	1.57968600	-2.60061900	-0.74773700
N	3.19529700	-1.21856900	0.09608500
C	2.93201200	-2.45419400	-0.29869000
C	4.42156600	-0.70879800	0.69037700
H	5.31657500	-1.27041500	0.39471700
H	4.32874400	-0.77379200	1.78343200
C	4.54410600	0.76884700	0.26712400
H	5.12261200	0.84499800	-0.66576200
H	5.08379400	1.34640000	1.03279800
O	-0.48254900	1.59106000	-0.79139800
O	-0.41707000	-1.51979300	-0.98591500
O	-0.40245000	-0.12209500	1.74994700
N	-3.09229300	1.34269300	0.98786400
N	-3.03994600	-1.47203800	0.77633700
N	-2.93814500	0.09221700	-1.68969900
C	-3.72662800	0.57047300	2.08836400
H	-3.43268800	1.00509000	3.04865800
H	-4.81823900	0.67266100	2.03420100
C	-3.31915700	-0.92041400	2.11603600
H	-4.10251300	-1.49777800	2.63866500
H	-2.39127400	-1.02299200	2.68245900
C	-3.84410600	-1.06818300	-1.56813200
H	-3.31307600	-1.91252600	-2.01752800
H	-4.77029700	-0.92305200	-2.15176900
C	-4.21505600	-1.44935300	-0.12286600
H	-4.70741100	-2.43353700	-0.14522700
H	-4.95722000	-0.75900300	0.27778000
C	-3.55033000	1.42432400	-1.50385100
H	-2.76515200	2.14422600	-1.74970400
H	-4.38478100	1.58342100	-2.21069200
C	-4.05425400	1.71568100	-0.08337100
H	-4.28267700	2.79017500	-0.02860900
H	-5.00421000	1.20514800	0.08874000
C	-2.47624200	-2.82854900	0.89152000
H	-1.55185600	-2.78129400	1.47092100
H	-3.18276200	-3.51821100	1.38359600
H	-2.22435100	-3.20454800	-0.10088100
C	-2.37701300	2.53083800	1.49780600
H	-1.86465500	3.01550600	0.66601800
H	-3.06317500	3.24161100	1.98770100
H	-1.61451800	2.20627000	2.20888100
C	-2.24212500	0.05709500	-2.99538100
H	-1.69106300	-0.88091000	-3.07728900
H	-2.94983700	0.15633000	-3.83508600
H	-1.51597600	0.87103700	-3.02206300
O	1.45724000	-0.20919200	2.81317900
C	2.90096300	2.51705300	-0.28498200
C	0.82090700	3.96329200	-0.95150200
H	0.09696500	4.24757900	-0.17648900
H	1.52514500	4.79015700	-1.07138000
H	0.25339100	3.85156200	-1.88233200
C	3.95334400	3.58883100	-0.37322500
H	4.71808200	3.33442800	-1.12128000
H	3.53102400	4.55596800	-0.65306800
H	4.47614400	3.72050700	0.58346700
C	0.94112800	-3.87520100	-1.21065100
H	1.67700800	-4.67740100	-1.31251700
H	0.16575600	-4.21273900	-0.51046700
H	0.44556100	-3.73001100	-2.17756200
C	3.91418000	-3.59679900	-0.28081800
H	3.63679900	-4.35475000	0.46395600
H	3.95727200	-4.10183400	-1.25318000
H	4.92426500	-3.25818800	-0.03899800
Mg	-1.40148800	-0.03402300	-0.05548000
Co	1.81513600	0.01975600	0.03630200
N	0.89561400	-0.10946400	1.73128900